

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 "Ask CAS" for self-help around the clock
NEWS 3 SEP 09 CA/CAPLUS records now contain indexing from 1907 to the present
NEWS 4 DEC 08 INPADOC: Legal Status data reloaded
NEWS 5 SEP 29 DISSABS now available on STN
NEWS 6 OCT 10 PCTFULL: Two new display fields added
NEWS 7 OCT 21 BIOSIS file reloaded and enhanced
NEWS 8 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 9 NOV 24 MSDS-CCOHS file reloaded
NEWS 10 DEC 08 CABA reloaded with left truncation
NEWS 11 DEC 08 IMS file names changed
NEWS 12 DEC 09 Experimental property data collected by CAS now available in REGISTRY
NEWS 13 DEC 09 STN Entry Date available for display in REGISTRY and CA/CAPLUS
NEWS 14 DEC 17 DGENE: Two new display fields added
NEWS 15 DEC 18 BIOTECHNO no longer updated
NEWS 16 DEC 19 CROPU no longer updated; subscriber discount no longer available
NEWS 17 DEC 22 Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18 DEC 22 IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19 DEC 22 ABI-INFORM now available on STN

NEWS EXPRESS DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS INTER General Internet Information
NEWS LOGIN Welcome Banner and News Items
NEWS PHONE Direct Dial and Telecommunication Network Access to STN
NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 10:19:30 ON 21 JAN 2004

=> **FILE reg**

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:19:59 ON 21 JAN 2004

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

DICTIONARY FILE UPDATES: 20 JAN 2004 HIGHEST RN 639777-15-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> e cu2sb

E1	1	CU2S8TL2ZR3/BI
E2	1	CU2S9SN4/BI
E3	1 -->	CU2SB/BI
E4	1	CU2SB0.5-1TL0-0.5/BI
E5	1	CU2SB2SR/BI
E6	1	CU2SB3U3/BI
E7	1	CU2SB7/BI
E8	3	CU2SBSE3/BI
E9	1	CU2SBTI/BI
E10	1	CU2SC/BI
E11	1	CU2SC0/BI
E12	1	CU2SC0.5SR2.5TLO7/BI

=> e cu2sb/mf

E1	1	CU2S8TL2ZR3/MF
E2	1	CU2S9SN4/MF
E3	1 -->	CU2SB/MF
E4	1	CU2SB0.5-1TL0-0.5/MF
E5	1	CU2SB2SR/MF
E6	1	CU2SB3U3/MF
E7	1	CU2SB7/MF
E8	1	CU2SBSE3/MF
E9	1	CU2SBTI/MF
E10	1	CU2SC/MF
E11	1	CU2SCSI2/MF
E12	4	CU2SE/MF

=> s e3

L1 1 CU2SB/MF

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 12054-21-6 REGISTRY
CN Antimony, compd. with copper (1:2) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Copper antimonide (Cu2Sb) (6CI, 7CI, 8CI)
CN Copper, compd. with antimony (2:1)
MF Cu . Sb
AF **Cu2 Sb**
CI TIS
LC STN Files: CA, CAOLD, CAPLUS, CHEMLIST, TOXCENTER, USPATFULL
Other Sources: EINECS**
(**Enter CHEMLIST File for up-to-date regulatory information)

Component	Ratio	Component Registry Number
Cu	2	7440-50-8
Sb	1	7440-36-0

122 REFERENCES IN FILE CA (1907 TO DATE)

122 REFERENCES IN FILE CAPLUS (1907 TO DATE)
24 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e cu2As/mf

E1	1	CU29O2/MF
E2	1	CU29S15/MF
E3	0 -->	CU2AS/MF
E4	1	CU2D/MF
E5	1	CU2D3/MF
E6	1	CU2D3NAO10S2/MF
E7	1	CU2D3NO6/MF
E8	1	CU2DY/MF
E9	1	CU2DY0.2GD0.8O8RUSR2/MF
E10	1	CU2DY0.4GD0.6O8RUSR2/MF
E11	1	CU2DY0.5O5Y1.5/MF
E12	1	CU2DY0.5O5YB1.5/MF

=> e asCu2/mf

E1	1	ASCU1.85EUSB/MF
E2	1	ASCU11FE4GES16/MF
E3	3 -->	ASCU2/MF
E4	1	ASCU2-4FE0-2S0-2SE2-4/MF
E5	1	ASCU2.4/MF
E6	1	ASCU2H2O6/MF
E7	1	ASCU2H3O6/MF
E8	1	ASCU2H3O6.XH2O/MF
E9	1	ASCU2HO5/MF
E10	1	ASCU2HO5.3H2O/MF
E11	1	ASCU2HO5.6H2O/MF
E12	1	ASCU2HO5.XH2O/MF

=> s e3

L2 3 ASCU2/MF

=> d 1-

YOU HAVE REQUESTED DATA FROM 3 ANSWERS - CONTINUE? Y/(N):y

L2 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
RN 303143-23-9 REGISTRY
CN Cuprate(1-), μ -arsenidodi- (9CI) (CA INDEX NAME)
MF **As Cu2**
CI CCS
SR CA
LC STN Files: CA, CAPLUS

Cu-As³⁻-Cu

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN

~~RN 12418-43-8~~ REGISTRY
CN Koutekite (Cu2As) (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Koutekite (7CI)
MF **As Cu2**
CI MNS, MAN
LC STN Files: CA, CAOLD, CAPLUS

STRUCTURE DIAGRAM IS NOT AVAILABLE

9 REFERENCES IN FILE CA (1907 TO DATE)
9 REFERENCES IN FILE CAPLUS (1907 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L2 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 12254-87-4 REGISTRY
 CN Copper arsenide (Cu₂As) (8CI, 9CI) (CA INDEX NAME)
 MF As . Cu
 AF As Cu₂
 CI TIS
 LC STN Files: CA, CAOLD, CAPLUS, IFICDB, IFIPAT, IFIUDB

Component	Ratio	Component Registry Number
Cu	2	7440-50-8
As	1	7440-38-2

12 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 12 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> e Cu₂P/mf

E1 1 CU2OTI4/MF
 E2 1 CU2OZR4/MF
 E3 1 --> CU2P/MF
 E4 1 CU2P2S2/MF
 E5 1 CU2P2S3/MF
 E6 1 CU2P2TH/MF
 E7 1 CU2P2U/MF
 E8 1 CU2P2YB/MF
 E9 1 CU2P2ZR/MF
 E10 1 CU2P7/MF
 E11 1 CU2P78PRW22.XH2O.17K/MF
 E12 1 CU2PB/MF

=> s e3

L3 1 CU2P/MF

=> d

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 12324-28-6 REGISTRY
 CN Copper phosphide (Cu₂P) (9CI) (CA INDEX NAME)
 MF Cu . P
 AF Cu₂ P
 CI TIS
 LC STN Files: CA, CAPLUS

Component	Ratio	Component Registry Number
P	1	7723-14-0
Cu	2	7440-50-8

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> help dir

The following HELP messages are available to obtain information on the REGISTRY File.

General Information:

<u>HELP ACCESSION</u>	-	REGISTRY accession number formats
<u>HELP CONTENT</u>	-	General REGISTRY File description
<u>HELP COST</u>	-	Price schedule for the REGISTRY File
<u>HELP DESK</u>	-	Information on REGISTRY File user assistance

General Search Information:

<u>HELP CASLINK</u>	-	Automated searches in the CASLINK cluster
<u>HELP CROSSOVER</u>	-	File crossover searching in REGISTRY
<u>HELP EFIELDS</u>	-	List of select field codes
<u>HELP FS</u>	-	File Segment searching in REGISTRY
<u>HELP HCASLINK</u>	-	Automated searches in the HCASLINK cluster
<u>HELP (L)</u>	-	(L) operator use in the REGISTRY File
<u>HELP LC</u>	-	CAS Registry Number Locator field
<u>HELP LIPINSKI</u>	-	Searching Lipinski property parameters
<u>HELP LLIMIT</u>	-	Limiting Search Codes for L-numbers
<u>HELP (P)</u>	-	(P) operator use in the REGISTRY File
<u>HELP RANGE</u>	-	RANGE parameters for the REGISTRY File
<u>HELP RNWEEK</u>	-	Highest RN on a weekly basis for the past year
<u>HELP RNYEAR</u>	-	Highest RN at the beginning of each year
<u>HELP (S)</u>	-	(S) operator use in the REGISTRY File
<u>HELP SFIELDS</u>	-	List of search field codes for general, nomenclature, and formula-based search terms
<u>HELP SLIMITS</u>	-	Structure search limits in the REGISTRY File
<u>HELP SPROJECTIONS</u>	-	Structure search projections for a FULL search based on SAMPLE search results
<u>HELP SREG</u>	-	List of sources of registration in the Source of Registration (SR) field
<u>HELP SRINGS</u>	-	List of ring data search fields
<u>HELP SRTFIELDS</u>	-	SORT command and SORT fields
<u>HELP STEREO</u>	-	Explanation of stereo messages
<u>HELP SUBSET</u>	-	SUBSET searching in the REGISTRY File
<u>HELP UPDATE/SDI</u>	-	Manual and automatic update searching
<u>HELP USAGETERM</u>	-	Use and distribution restrictions applicable to the REGISTRY File

Display Information:

<u>HELP DFIELDS</u>	-	List of display field codes
<u>HELP DIAGRAM</u>	-	Structure diagrams
<u>HELP DNLDFORMATS</u>	-	Formats for the DOWNLOAD command
<u>HELP DSCAN</u>	-	List of display fields shown in DISPLAY SCAN
<u>HELP FORMAT</u>	-	Predefined formats for DISPLAY and PRINT
<u>HELP HIGHLIGHTING</u>	-	Highlighting in the REGISTRY File

Information about Sequence Searching:

<u>HELP AAC</u>	-	1- and 3-letter codes for common amino acids
<u>HELP AAU</u>	-	3-letter codes for uncommon amino acids
<u>HELP BLAST</u>	-	BLAST similarity searching in Registry
<u>HELP NUC</u>	-	Codes for nucleic acids
<u>HELP SSQ</u>	-	Sequence search methods and fields
<u>HELP SQLINK</u>	-	Sequence linking with SEQLINK
<u>HELP SQQ</u>	-	Variability symbols in subsequence queries

Information about Polymer Searching:

<u>HELP PCT</u>	-	Polymer classes
<u>HELP PLINK</u>	-	Polymer registration and the POLYLINK command

Information about Property Searching:

<u>HELP ACD</u>	-	Definitions of ACD properties in REGISTRY
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<u>HELP CALC</u>	- Calculated property information in REGISTRY
<u>HELP DUNITS</u>	- Specifying units for display fields
<u>HELP CAPROP</u>	- Definitions of CAS collected properties
<u>HELP EPROP</u>	- Experimental property information in REGISTRY
<u>HELP IC</u>	- Definitions of InfoChem properties in REGISTRY
<u>HELP PROPERTIES</u>	- Overview of property information in REGISTRY
<u>HELP QRD</u>	- Query-Related Data in displays and prints
<u>HELP SNUMERIC</u>	- Numeric fields and how to search them
<u>HELP SUNITS</u>	- Specifying units for search fields
<u>HELP UNITS</u>	- Where to see units for properties in the REGISTRY File

Information about Regulatory Listings:

<u>HELP DSL/NDSL</u>	- Substances with the DSL or NDSL LC flag
<u>HELP EINECS</u>	- Substances with the EINECS LC flag
<u>HELP TSCA</u>	- Substances with the TSCA LC flag
<u>HELP WHO</u>	- Substances with the WHO flag

Information about Alloys:

<u>HELP ALLOY</u>	- Alloy searching in REGISTRY
<u>HELP MAC</u>	- Searching alloy weight percent composition data
<u>HELP RC</u>	- Searching alloy relative composition data

Information about Manual Registrations:

<u>HELP MAN/CI</u>	- Information about manual registrations
<u>HELP RN*</u>	- Information on RNs with asterisks (*)

For a list of more general help topics such as command usage, enter HELP MESSAGES at an arrow prompt (=>).

=> **help efields**

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms set taken from the specified field in an answer set.

The keyword, HIT, may be used in the SELECT and ANALYZE commands to restrict the terms extracted from the displayed data to terms that match the search expression used to create the answer set. The HIT keyword functions only if the answer set was created with HIGHLIGHTING ON. The resulting list of terms are the hit terms in the specified field.

Example (to create E-numbers):

```
=> S DIOXIN/CN
L1          2 DIOXIN/CN

=> SELECT L1
ENTER ANSWER NUMBER OR RANGE (1-):.
ENTER DISPLAY CODE (CHEM) OR ?:CN
E1 THROUGH E25 ASSIGNED

=> D SEL
E1          2      DIOXIN/CN
E2          1      ACETOMETHOXANE/CN
E3          1      AROMATIC HYDROCARBON RECEPTOR (HUMAN CLONE
                   HU14)/CN
E4          1      DIBENZO(B,E) (1,4)DIOXIN, 2,3,7,8-
```

```

          TETRACHLORO-/CN
E5        1  DIBENZO-P-DIOXIN, 2,3,7,8-TETRACHLORO-/CN
E6        1  DIMETHOXANE/CN
E7        1  DIOXIN (BACTERICIDE)/CN
E8        1  DIOXIN (HERBICIDE CONTAMINANT)/CN
E9        1  DIOXIN CO/CN
E10       1  GIV GARD DXN-CO/CN
E11       1  GIV GARD DXN/CN
E12       1  M-DIOXAN-4-OL, 2,6-DIMETHYL-, ACETATE/CN
E13       1  TCDBD/CN
E14       1  TCDD/CN
E15       1  1,3-DIOXAN-4-OL, 2,6-DIMETHYL-, ACETATE/CN
E16       1  2,3,7,8-TCDD/CN
E17       1  2,3,7,8-TETRACHLORODIBENZO(B,E)(1,4)DIOXIN/CN
E18       1  2,3,7,8-TETRACHLORODIBENZO-P-DIOXIN/CN
E19       1  2,3,7,8-TETRACHLORODIBENZO-1,4-DIOXIN/CN
E20       1  2,4-DIMETHYL-6-ACETOXY-1,3-DIOXANE/CN
E21       1  2,4-DIMETHYL-6-M-DIOXANYL ACETATE/CN
E22       1  2,6-DIMETHYL-M-DIOXAN-4-OL ACETATE/CN
E23       1  2,6-DIMETHYL-M-DIOXAN-4-YL ACETATE/CN
E24       1  6-ACETOXY-2,4-DIMETHYL-M-DIOXANE/CN
E25       1  6-ACETOXY-2,4-DIMETHYL-1,3-DIOXANE/CN

```

Example (to create an L-number):

```

=> S DIOXIN/CN
L1        2 DIOXIN/CN

=> ANALYZE L1
ENTER ANSWER NUMBER OR RANGE (1-):.
ENTER DISPLAY CODE (CHEM) OR ?:CN
L2        ANALYZE L1 1- CN :      25 TERMS

```

```

=> D

L2        ANALYZE L1 1- CN :      25 TERMS

```

TERM #	# OCC	# DOC	% DOC	CN
1	2	2	100.00	DIOXIN
2	1	1	50.00	ACETOMETHOXANE
3	1	1	50.00	AROMATIC HYDROCARBON RECEPTOR (HUMAN CLONE HU
4	1	1	50.00	DIBENZO(B,E)(1,4)DIOXIN, 2,3,7,8-TETRACHLORO-
5	1	1	50.00	DIBENZO-P-DIOXIN, 2,3,7,8-TETRACHLORO-
6	1	1	50.00	DIMETHOXANE
7	1	1	50.00	DIOXIN (BACTERICIDE)
8	1	1	50.00	DIOXIN (HERBICIDE CONTAMINANT)
9	1	1	50.00	DIOXIN CO
10	1	1	50.00	GIV GARD DXN-CO

15 MORE TERMS WITH AN OCCURRENCE COUNT OF 1

The display fields from which terms may be extracted in the REGISTRY File are listed below.

Display Code	Definition
AF	Alternate Molecular Formula
AR	Alternate CAS Registry Number
CCI	Component Class Identifier (appends /CI to terms created by SELECT)

CHEM	CAS Registry Numbers and Names (default) (appends /BI to terms created by SELECT)
CI	Class Identifier
CMF	Component Molecular Formula (appends /BI to terms created by SELECT)
CN	Chemical Names (Up to 50)
CRN	Component CAS Registry Number
DR	Deleted CAS Registry Number
DEF	Definition
ED	Entry Date
ENTE	Editor Note
FCN	All Chemical Names
FS	File Segment
IN	CA Index Name
LC	CAS Registry Number Locator (extracts the files with searchable CAS Registry Numbers that contain information on the Registry Number of the record. E-numbers may be used in the in the FILE and INDEX commands to enter the files selected.)
MF	Molecular Formula
NAME	Names (appends /BI to terms created by SELECT)
PCT	Polymer Class Term
PR	Preferred CAS Registry Number
RN	CAS Registry Number (appends /BI to terms created by SELECT))
RR	Replacing CAS Registry Number
SCN	Short Chemical Name (extracts IN and OTHER NAMES with /CN appended to terms created by SELECT)
SR	Source of Registration

Ring Analysis Fields

EA	Elemental Analysis for Ring System
ES	Elemental Sequence for Ring System
RID	Ring Identifier
SZ	Size for Ring System
RF	Ring System Formula

Sequence Fields

PN	-----	Patent number from the PNTE (Patent Annotation) field
SEQ	-----	Protein Sequence (1-letter amino acid codes - /SQSP appended to terms created by SELECT)
SEQ3	----	Protein Sequence (3-letter amino acid codes - /SQSP appended to terms created by SELECT)

Additional codes are available for extracting sequences to be used in the various types of sequence searches:

SQEN	----	Nucleic Acid Sequence (exact search form - /SQEN appended to terms created by SELECT)
SQEFPP	---	Protein Sequence (exact family search form - /SQEFPP appended to terms created by SELECT)
SQEP	----	Protein Sequence (exact search form - /SQEP appended to terms created by SELECT)
SQSN	----	Nucleic Acid Sequence (subsequence search form - /SQSN appended to terms created by SELECT)
SQSFP	---	Protein Sequence (subsequence family search form - /SQSFP appended to terms created by SELECT)
SQSP	----	Protein Sequence (subsequence search form - /SQSP appended to terms created by SELECT)

SELECT CHEM or ANALYZE CHEM may be used to extract the RN, DR, AR, PR and Chemical Name (CN, except for inverted CA Index Names) display fields in the REGISTRY File. If you wish to extract only the

substance names, you use SELECT NAME or ANALYZE NAME. The /BI field code will be appended to terms created by SELECT.

Additional information on DR, AR, and PR is available in HELP ACCESSION.

=> d hist

(FILE 'HOME' ENTERED AT 10:19:30 ON 21 JAN 2004)

FILE 'REGISTRY' ENTERED AT 10:19:59 ON 21 JAN 2004

```

      E CU2SB
      E CU2SB/MF
L1    1 S E3
      E CU2AS/MF
      E ASCU2/MF
L2    3 S E3
      E CU2P/MF
L3    1 S E3
```

=> e Cu1.9Sb

```

E1    1      CU1.9O7V2ZN0.1/BI
E2    1      CU1.9S/BI
E3    0 --> CU1.9SB/BI
E4    1      CU1.9SE/BI
E5    1      CU1.9SRZN0.1O3/BI
E6    1      CU1.9TE/BI
E7    1      CU1.9TE3ZR/BI
E8    1      CU1.9V12O29/BI
E9    1      CU1.9V2ZN0.1O7/BI
E10   1      CU1.9Y2ZN0.1O5/BI
E11   1      CU1.9ZRTE3/BI
E12   14     CU10/BI
```

=> e cu2.1sb/mf

```

E1    1      CU2.1O7.9RU0.9SR2Y/MF
E2    1      CU2.1O8RU0.9SR2/MF
E3    0 --> CU2.1SB/MF
E4    1      CU2.2 FE0.8 O6 SR2 Y/MF
E5    1      CU2.2 FE0.8 O6.98 SR2 Y/MF
E6    1      CU2.2 FE0.8 O7 SR2 Y/MF
E7    1      CU2.2 FE2.2 TE2/MF
E8    1      CU2.2 GA0.8 O7 SR2 Y/MF
E9    1      CU2.2 GD O8 RU0.8 SR2/MF
E10   1      CU2.2 HG0.8 SN TE4/MF
E11   1      CU2.2 IN SE2/MF
E12   1      CU2.2 LA SI2/MF
```

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	30.54	30.75

FILE 'CAPLUS' ENTERED AT 10:31:41 ON 21 JAN 2004

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 21 Jan 2004 VOL 140 ISS 4
FILE LAST UPDATED: 20 Jan 2004 (20040120/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 11-13

122 L1
23 L2
1 L3
L4 146 (L1 OR L2 OR L3)

=> s 14 and anode

119729 ANODE
L5 7 L4 AND ANODE

=> d ibib ab it 1-

YOU HAVE REQUESTED DATA FROM 7 ANSWERS - CONTINUE? Y/(N):y

L5 ANSWER 1 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Citing
References

ACCESSION NUMBER: 2003:672274 CAPLUS
DOCUMENT NUMBER: 139:389068
TITLE: Lithiation of InSb and Cu₂Sb: a theoretical investigation
AUTHOR(S): Sharma, S.; Dewhurst, J. K.; Ambrosch-Draxl, C.
CORPORATE SOURCE: Inst. for Theor. Phys., Karl-Franzens-Univ. Graz, Graz, A-8010, Austria
SOURCE: Los Alamos National Laboratory, Preprint Archive, Condensed Matter (2003) 1-5, arXiv:cond-mat/0308546, 26 Aug 2003
CODEN: LNCMFR
URL: <http://xxx.lanl.gov/pdf/cond-mat/0308546>
PUBLISHER: Los Alamos National Laboratory
DOCUMENT TYPE: Preprint
LANGUAGE: English

AB In this work the mechanism of Li insertion/intercalation in the **anode** materials InSb and Cu₂Sb is investigated by means of the first principles total energy calcns. The total charge densities for the lithiated products of the two compds. are presented. Based on these results the change in the bonding character on lithiation is discussed. Further, the isomer shift for InSb and Cu₂Sb and there various lithiated products is reported. The av. insertion/intercalation voltage and vol. expansion for transitions from InSb to Li₂InSb and Cu₂Sb to Li₂CuSb are calcd. and found to be in good agreement with the exptl. values. These findings help to resolve the controversy regarding the lithiation mechanism in InSb.

IT Isomers
(positional; theor. investigation of lithiation of InSb and Cu₂Sb)

IT Anodes
Bond
Intercalation
Lithiation
Quantum chemistry
Total energy

(theor. investigation of lithiation of InSb and Cu₂Sb)
IT 12324-21-9 620177-89-1

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(theor. investigation of lithiation of InSb and Cu₂Sb)

IT 1312-41-0, Indium antimonide 7439-93-2, Lithium, processes
12054-21-6

RL: PEP (Physical, engineering or chemical process); PYP (Physical process); PROC (Process)

(theor. investigation of lithiation of InSb and Cu₂Sb)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Cited
References

ACCESSION NUMBER: 2002:950103 CAPLUS

DOCUMENT NUMBER: 138:323783

TITLE: Structural considerations of intermetallic electrodes for lithium batteries

AUTHOR(S): Thackeray, M. M.; Vaughey, J. T.; Johnson, C. S.; Kropf, A. J.; Benedek, R.; Fransson, L. M. L.; Edstrom, K.

CORPORATE SOURCE: Chemical Technology Division, Electrochemical Technology Program, Argonne National Laboratory, Argonne, IL, 60439, USA

SOURCE: Journal of Power Sources (2003), 113(1), 124-130
CODEN: JPSODZ; ISSN: 0378-7753

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review. Although metal alloys and intermetallic compds. have been researched extensively as possible neg. electrodes for lithium batteries, only recently have efforts been made to monitor the phase transitions that occur during their reaction with lithium by in situ X-ray diffraction. These studies have lead to attempts to exploit those systems that show strong structural relationships between a parent structure and its lithiated products. In this paper, an overview of several systems is presented, particularly those that operate by lithium insertion/metal displacement reactions with a host metal array at room temp. An analogy between these reactions and the high-temp. electrochem. reaction of sodium/nickel chloride cells, which is 100% efficient, is provided. On this basis, a prognosis for using intermetallic electrodes in lithium-ion cells is given.

IT Secondary batteries
(lithium; structural considerations of intermetallic electrodes for lithium batteries)

IT Battery anodes
(structural considerations of intermetallic electrodes for lithium batteries)

IT Intermetallic compounds
RL: DEV (Device component use); PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process); USES (Uses)

(structural considerations of intermetallic electrodes for lithium batteries)

IT 7439-93-2, Lithium, processes

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(structural considerations of intermetallic electrodes for lithium batteries)

IT 1312-41-0 12019-69-1 12032-82-5 12054-21-6 28980-49-6

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)

(structural considerations of intermetallic electrodes for lithium batteries)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Full Text	Citing References
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ACCESSION NUMBER: 2002:736749 CAPLUS
 DOCUMENT NUMBER: 137:265676
 TITLE: Intermetallic anodes for lithium cells and batteries
 INVENTOR(S): Vaughey, John T.; Fransson, Linda M. L.; Thackeray, Michael M.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 17 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002136953	A1	20020926	US 2002-68230	20020204
PRIORITY APPLN. INFO.:		US 2001-267512P P 20010208		
AB	A neg. electrode is disclosed for a nonaq. electrochem. cell. The electrode has an intermetallic compd. as its basic structural unit with the formula M ₂ M' in which M and M' are selected from two or more metal elements including Si, and the M ₂ M' structure is a Cu ₂ Sb-type structure. Preferably M is Cu, Mn and/or Li, and M' is Sb. Also disclosed is a nonaq. electrochem. cell having a neg. electrode of the type described, an electrolyte and a pos. electrode. A plurality of cells may be arranged to form a battery.			
IT	Ball milling Battery anodes (intermetallic anodes for lithium cells and batteries)			
IT	Intermetallic compounds RL: DEV (Device component use); USES (Uses) (intermetallic anodes for lithium cells and batteries)			
IT	Secondary batteries (lithium; intermetallic anodes for lithium cells and batteries)			
IT	12032-97-2P 12054-21-6P 12057-30-6P 12324-21-9P 461642-86-4P 461642-87-5P 461642-88-6P RL: DEV (Device component use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (intermetallic anodes for lithium cells and batteries)			
IT	7782-42-5, Graphite, uses RL: TEM (Technical or engineered material use); USES (Uses) (solid lubricant; intermetallic anodes for lithium cells and batteries)			

Full Text	Citing References
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ACCESSION NUMBER: 2001:465014 CAPLUS
 DOCUMENT NUMBER: 135:229274
 TITLE: Phase transitions in lithiated Cu₂Sb anodes for lithium batteries: an in situ X-ray diffraction study
 AUTHOR(S): Fransson, L. M. L.; Vaughey, J. T.; Benedek, R.; Edstrom, K.; Thomas, J. O.; Thackeray, M. M.
 CORPORATE SOURCE: Department of Materials Chemistry, Angstrom Laboratory, Uppsala University, Swed.
 SOURCE: Electrochemistry Communications (2001), 3(7), 317-323
 CODEN: ECCMF9; ISSN: 1388-2481
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Copper antimonide, Cu₂Sb, has been investigated as a neg. electrode (anode) for rechargeable lithium batteries by in situ X-ray diffraction of Li/Cu₂Sb cells. The data show that lithium is inserted into Cu₂Sb with a concomitant extrusion of copper, which initiates a phase transition to a

lithiated zinc-blende-type structure, $\text{Li}_x\text{Cu}_{2-y}\text{Sb}$ for $0 < x \leq 2$ and $0 \leq y \leq 1$, yielding Li_2CuSb at $x = 2$, $y = 1$. Further lithiation results in the displacement of the remaining copper to yield $\text{Li}_{2+z}\text{Cu}_{1-z}\text{Sb}$ compns. ($0 < z \leq 1$) with the end member Li_3Sb . The Sb array remains intact in a face-centered arrangement throughout these reactions, despite a 42% expansion of the array. The reactions are reversible; they occur between 1.0 and 0 V vs. Li_0 , and deliver a steady capacity of approx. 290 mAh/g after one conditioning cycle. The lithium insertion/metal extrusion reactions with the Cu_2Sb structure bear a resemblance to those obsd. previously with Cu_6Sn_5 and InSb .

- IT Phase transition
(in lithiated Cu_2Sb anodes for lithium batteries, an in situ X-ray diffraction study)
- IT Secondary batteries
(lithium; phase transitions in lithiated Cu_2Sb anodes for lithium batteries, an in situ X-ray diffraction study)
- IT Anodes
(phase transitions in lithiated Cu_2Sb anodes for lithium batteries, an in situ X-ray diffraction study)
- IT **12054-21-6**, Copper antimonide (Cu_2Sb)
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(phase transitions in lithiated Cu_2Sb anodes for lithium batteries, an in situ X-ray diffraction study)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

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Text

ACCESSION NUMBER: 1995:305167 CAPLUS
DOCUMENT NUMBER: 122:60155
TITLE: Secondary high-temperature battery and its manufacture
INVENTOR(S): Coetzer, Johan; Vlok, Isak Louw
PATENT ASSIGNEE(S): Programme 3 Patent Holdings, Luxembourg
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9423467	A2	19941013	WO 1994-EP1027	19940331
WO 9423467	A3	19941124		
W: AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, FI, GB, GE, HU, JP, KG, KP, KR, KZ, LK, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5368955	A	19941129	US 1994-215844	19940322
ZA 9402048	A	19941003	ZA 1994-2048	19940323
AU 9465642	A1	19941024	AU 1994-65642	19940331
EP 693228	A1	19960124	EP 1994-913511	19940331
EP 693228	B1	19970827		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
JP 08506928	T2	19960723	JP 1994-521680	19940331
AT 157484	E	19970915	AT 1994-913511	19940331
ES 2107210	T3	19971116	ES 1994-913511	19940331
FR 2703513	A1	19941007	FR 1994-3891	19940401
FR 2703513	B1	19950804		
US 5476733	A	19951219	US 1994-344651	19941118
PRIORITY APPLN. INFO.:			ZA 1993-2406	A 19930402

ZA 1993-2650	A 19930415
ZA 1993-3459	A 19930518
ZA 1993-9121	A 19931206
ZA 1993-1215	A 19931206
US 1994-215844	B1 19940322
WO 1994-EP1027	A 19940331

AB The battery has a molten Na anode sepd. by Na ion-conducting solid electrolyte separator from a solid cathode comprising an electronically conductive electrolyte-permeable porous matrix. The matrix is impregnated with a molten salt electrolyte and contains dispersed solid active cathode material. The electrolyte comprises a substantially equimolar mixt. of NaCl and AlCl₃. The active cathode material comprises ≥ 1 transition metal selected from Fe, Ni, Cr, Co, Mn, Cu, and Mo. At least 1 additive element selected from As, Bi, Sb, Se, and Te is dispersed in the active cathode material, the at. ratio of transition metal:additive element being 99:10-30:70. The active cathode material in the charged state of the battery is chlorinated.

IT Batteries, secondary

(sodium-transition metal chloride high-temp.)

IT 11088-65-6, Copper antimonide (CuSb) 12022-92-3, Iron antimonide (FeSb) 12022-93-4, Iron antimonide (FeSb₂) 12035-52-8, Nickel antimonide (NiSb) 12035-53-9, Nickel antimonide (NiSb₂) 12054-21-6, Copper antimonide (Cu₂Sb) 12503-49-0, Nickel antimonide (Ni₃Sb) 12503-51-4, Nickel antimonide (Ni₅Sb₂) 12503-54-7, Nickel antimonide (Ni₇Sb₃) 27016-75-7, Nickel arsenide (NiAs) 160351-69-9
RL: DEV (Device component use); USES (Uses)

(cathode in high-temp. sodium battery)

IT 7439-89-6, Iron, uses 7439-96-5, Manganese, uses 7439-98-7, Molybdenum, uses 7440-02-0, Nickel, uses 7440-47-3, Chromium, uses 7440-48-4, Cobalt, uses 7440-50-8, Copper, uses
RL: DEV (Device component use); USES (Uses)

(dispersed additive element-contg. transition metal cathode for high-temp. sodium battery)

IT 7647-15-6, Sodium bromide, uses 7681-82-5, Sodium iodide, uses 7772-99-8, Tin dichloride, uses

RL: MOA (Modifier or additive use); USES (Uses)

(dopant in cathode compartment of high-temp. sodium battery)

IT 7440-36-0, Antimony, uses 7440-38-2, Arsenic, uses 7440-69-9, Bismuth, uses 7782-49-2, Selenium, uses 13494-80-9, Tellurium, uses

RL: MOA (Modifier or additive use); USES (Uses)

(high-temp. sodium battery cathode of transition metal contg. dispersed)

L5 ANSWER 6 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

Full
Text

Citing
References

ACCESSION NUMBER: 1981:432589 CAPLUS
DOCUMENT NUMBER: 95:32589
TITLE: Copper and arsenic removal from a copper solution
PATENT ASSIGNEE(S): Nippon Mining Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 56020185	A2	19810225	JP 1979-93706	19790725
JP 57040231	B4	19820826		
PRIORITY APPLN. INFO.:			JP 1979-93706	19790725

AB A soln. from Cu electrefining contg. Cu and As is simultaneously stripped of Cu and As by codepositing Cu and As by electrolysis after converting all of the As to the trivalent state. Thus, a soln. contg. Ni

15, H2SO4 400, Cu 1-10, and As 1-8 g/L was electrolyzed using a Cu cathode, a Pb **anode**, a cathodic potential of -200 mV, bath temp. 30-33°, electrolysis time 2 h, and stirring with N gas. The Cu as As copptd. as Cu2As and Cu3As (a small amt.).

IT 7440-50-8P, preparation

RL: PREP (Preparation)
(electrorefining of, arsenic removal in)

IT 12005-75-3P **12254-87-4P**

RL: PREP (Preparation)
(formation of, electrochem., in arsenic removal in copper electrorefining)

IT 7440-38-2, uses and miscellaneous

RL: REM (Removal or disposal); PROC (Process)
(removal of, in copper electrorefining)

L5 ANSWER 7 OF 7 CAPLUS COPYRIGHT 2004 ACS on STN

Full Text Citing References

ACCESSION NUMBER: 1969:63590 CAPLUS
DOCUMENT NUMBER: 70:63590
TITLE: Electrolytic preparation of semiconductor compounds
INVENTOR(S): Ammerman, Frank E.; Schindehette, Donald J.
PATENT ASSIGNEE(S): Chrysler Corp.
SOURCE: U.S., 8 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3419484	A	19681231	US 1966-536624	19660323
PRIORITY APPLN. INFO.:			US 1966-536624	19660323

AB A process is described for the production of chem. compds. by electrosynthesis in which ions of the components elements of the desired compds. are reduced either by electrolysis of a soln. using electrodes and an external current source or by means of immersion or contact deposition in which electrons are generated within the soln. It consists of forming a soln. or bath contg. cations of the component elements of the compd. The soln. is then supplied with electrons with the result that the compd. is formed and deposited on 8the immediate electron source. The electrons can be supplied from an external source as by passing current between electrodes, or the electrons can be generated in the soln. as by immersion deposition or contact deposition. The compds. which can be formed by the process are those composed of at least one of the semimetals As, Te, or Sb and the other element any substance which has deposition potential less noble than that of the semimetal when both are in the soln. Conditions under which the process is carried out are not crit. E.g., CuTe is prepd. as follows. An aq. soln. is prepd. contg. CuCN 2, NaCN 3, NaOH 3, and TeO2 5 g. in 100 g. H2O. The TeO2 is 1st dissolved in a portion of the NaOH and H2O and then combined with the balance of the soln. The soln. is then electrolyzed at room temp. using a Cu **anode** and a steel cathode and a c.d. of ~10 amp./ft.2 A material is deposited at the cathode and anal. discloses it to be CuTe with residual traces of Te. Other compds., e.g., PbTe, HgTe, NiTe2, SnTe, Bi2Te3, AgTe, TlTe, Cu2As, etc. are similarly prepared.

IT Semiconductors, electric

(electrolytic manuf. of)

IT Iodide, uses and miscellaneous

RL: USES (Uses)
(doping with, of lead telluride)

IT Copper antimonide (CuSb2)

Lead selenide telluride (Pb2SeTe)
Palladium telluride (PdTe)

Thallium antimonide (Tl7Sb2)
 RL: PROC (Process)
 (electrolytic manuf. of)

IT 1303-00-0P, preparation
 RL: PREP (Preparation)
 (by electrolysis)

IT 7440-66-6, uses and miscellaneous
 RL: USES (Uses)
 (doping with, of lead telluride)

IT 1303-11-3P 1304-82-1P 1314-91-6P 12002-99-2P 12006-15-4P
12019-23-7P 12035-53-9P 12035-59-5P 12040-02-7P 12052-42-5P
12067-00-4P 12068-90-5P 12125-63-2P 12165-81-0P 12255-80-0P
12255-99-1P 14176-81-9P 28980-49-6P
 RL: PREP (Preparation)
 (electrolytic manuf. of)

IT 12040-12-9P **12254-87-4P**
 RL: PREP (Preparation)
 (in electrolytic manuf. of)

IT 1314-91-6P
 RL: PREP (Preparation)
 (iodide-contg., electrolytic manuf. of)

IT 1314-91-6P
 RL: PREP (Preparation)
 (zinc-contg., electrolytic manuf. of)

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